

Table S1. Twenty non-specific metabolites removed before metabolite set extension.

Metabolite	ChEBI	KEGG	PubChem
H ₂ O	15377	C00001	962
O ₂	15379	C00007	977
H ⁺	15378	C00282	1038
CO ₂	16526	C00011	280
HPO ₄ ²⁻	43474	C00009	1004
ATP	15422	C00002	5957
dATP	16284	C00131	15993
ADP	16761	C00008	6022
dADP	16174	C00206	188966
AMP	16027	C00020	6083
dAMP	17713	C00360	12599
Diphosphate	29888	C00013	1023
Nicotinamide adenine dinucleotide phosphate - reduced	57783	C00005	22833512
Nicotinamide adenine dinucleotide phosphate	18009	C00006	5886
Nicotinamide adenine dinucleotide - reduced	16908	C00004	439153
Nicotinamide adenine dinucleotide	15846	C00003	5893
Flavin adenine dinucleotide oxidized	16238	C00016	643975
Flavin adenine dinucleotide reduced	17877	C01352	446013
Coenzyme A	15346	C00010	6816
Hydrogen peroxide	16240	C00027	784

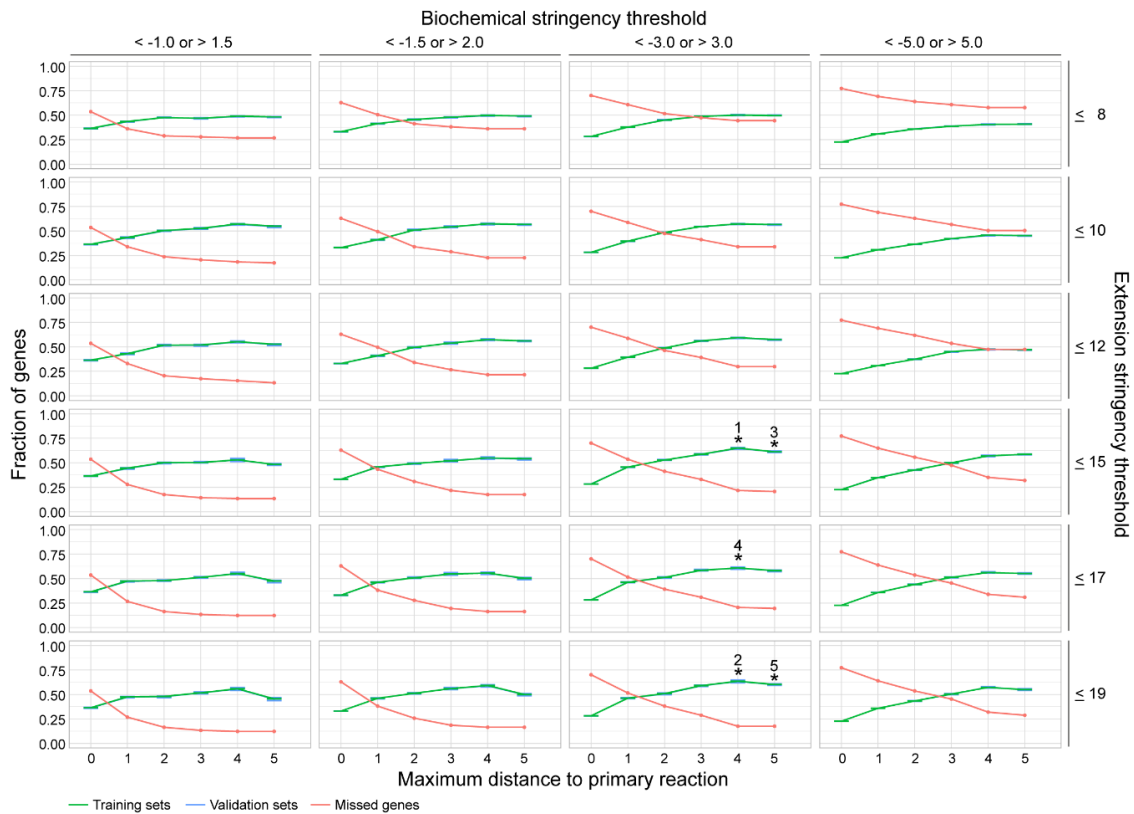


Figure S1. Assessment of the most favorable parameter combination of the cross-omics method in the ten test and validation sets. The diagnostic value of the cross-omics method for the different parameter combinations in the validation sets is depicted in blue, the diagnostic value in the test sets is depicted in green (overlying the blue lines), and the fraction of missed disease-causing genes is depicted in red. The five parameter combinations reaching the highest diagnostic value are highlighted with numbered asterisks: 1: 0.65; 2: 0.64; 3: 0.61; 4: 0.61; 5: 0.60).